4-Nitrosodiphenylamine 156-10-5 | DTXSID1021031

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 2.99

Global applicability domain: Inside

Local applicability domain index: 4.73e-01

Confidence level: 6.19e-01

Nearest Neighbors from the Training Set

Image not found 4,4'-Oxydianiline Measured: 1.36 Predicted: 1.57 Image not found 4-Anilinophenol Measured: 2.82 Predicted: 2.88 Image not found

Benzamide, N-(4-chlorophenyl)-

2-hydroxy-Measured: 4.50 Predicted: 3.86